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13. ABSTRACT (Maximum 200 Words)

This report summarizes the research work conducted during the period funded by the AFOSR grant. The PI has conducted a series of research projects on (a). development of hydrodynamic theories for inhomogeneous nematic liquid crystal polymers, cholesteric liquid crystals, blends of liquid crystal polymers and flexible polymer solutions or melts, biaxial liquid crystal polymers or suspension flows of biaxial nano-particles; (b). studies of nematodynamics as well as morphology of inhomogeneous nematic liquid crystal flows as well as relevant temporal chaotic and spatial chaotic behavior in the fascinating high performance material; (c). development of an effective theory to characterize the effective material properties for the nano-suspension and/or liquid crystal polymer; (d). studies of coupled flow and magnetic and electric field assisted processing for liquid crystal polymers as well as suspension flows. These subprojects have revealed a great deal of the flow-orientation couple dynamic in the flowing materials leading to some potential applications in the military and industries.

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Final Technical Report to AFOSR

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This report summarizes the work conducted during the period of Jan. 1, 2002 to March 31, 2005. During the grant-supported period, the PI continues to work on modeling and computation of flows of liquid crystal polymers (LCPs) and nanocomposites guided by Air Force contact Dr. Richard Vaia of material directorate WPAFB. The activities include developing kinetic theories for uniaxial molecules with finite extensibility, flows of cholesterics, nonhomogeneous flows accounting for stress induced polymer migration, as well as theories for biaxial liquid crystals and nano-particle suspension flows. A continuum theory for flow of cholesteric liquid crystals is also derived to explore the mesostructure in weak flows. Works on nematic rigid polymers are refined with the kinetic theory calculations. Materials properties for nanocomposites are explored through homogenization techniques using our mesoscopic structure calculations and an effective medium theory. The main collaborators in this period are Prof. M. G. Forest of UNC Chapel Hill, Prof. Ruhai Zhou (former Postdoc at UNC and now at Old Dominion), Prof. Bechtel of Ohio State University, Professor M C Calderer of University of Minnesota, Prof. Hong Zhou of Naval Post Graduate School, Prof. Rob lipton of LSU, and my graduate students Zhenlu Cui and Sarthok Sircar of FSU. (Zhenlu Cui has graduated this summer with a Ph. D. degree in mathematics.) In the following, I summarize the completed work and the work-in-progress briefly and list the publications within the period. For details, please refer to our publications.

Multiscale modeling and study of flow-orientation coupling in the shear flow of liquid crystal polymers.

The Pi and his collaborators (M. G. Forest and R. Zhou) continue refined analysis on the extended Doi-Hess kinetic theory for mondomain shear flows and general planar linear flows of liquid crystal polymers. The aim here is to provide a comprehensive understanding of the monodomain flow behavior governed by the kinetic theory. In a series of papers, we thoroughly examined the monodomain dynamics and characterized completely the complex dynamics governed by the kinetic theory using a Galerkin method based on the spherical harmonic expansions and a mesoscopic closure model. In the dilute regime, we solved the governing equation asymptotically in the weak shear limit and give the explicit scaling behavior of the solution with respect to the important

flow parameters as well as the geometric parameters of the molecules. The comprehensive phase diagram obtained using both closure and kinetic theory provides an atlas for further studies of the nonhomogeneous flow behavior of LCPs. Following the monodomain road map, we have identified a variety of temporal-spatial structures and patterns in sheared nematic LCPs of nonhomogeneous flows. The newly identified chaotic behavior in monodomain is also observed in the nonhomogeneous flow through both temporal and spatial ramifications.

In additional to the sheared nematic LCPs, we also examined the kinetic theory in general linear flows and discovered that the flow map can be completely recovered from our results for sheared nematics. The crucial link is the extended geometry parameter a. In other words, the general linear flow, including the important 4-roll-mills, can be obtained by rescaling the results for the sheared nematics. In two papers, we explored the basins of attractors and the chaotic boundaries using kinetic and closure models, respectively. The results are published in PRL and Rheological Acta, respectively.

Our current activities in this direction are (i). summarize our extensive results with respect to the nonhomogeneous mesoscopic structure and have them published and to compute the governing equation obtained via closures in multidimensional geometry aiming at understanding the flow-orientation interaction in sheared nonhomogeneous nematics and how the temporal structure in the monodomain interact with the spatial degree of freedom. Ref [3-6,9-11,13,18,20,24,25,33].

Multiscale models for uniaxial molecules of finite extensibility and nonhomogeneous liquid crystal polymers.

The kinetic theory developed in (Wang, 2002) has been extended to account for the spatial inhomogeneity of the lcp by allowing the density of the material to vary in space (Q Wang, M G Forest, and R Zhou, 2004). This additional degree of freedom is amount to introduce another order parameter for the spatial distribution of the center of mass of the liquid crystal polymers. Some spatial patterns related to the center of mass variation are therefore plausible. Indeed, we can solve the governing equations in the moment-averaged approximation to show that a periodic density pattern may form while the averaged molecular orientation is attained absent of flows. The potential layering is naturally built into the kinetic theory. We remark that the density variation of LCPs is not modeled in the classical theory of Ericksen-Leslie or any other continuum mechanical theories nor in the phenomenological theories of Tsuji-Rey's etc. In our most recent studies, we found the spatial variation of densities and the associated translational diffusion is intrinsically related to the long-range elastic distortion of the molecular orientation.

Lately, the theory is further refined to include the stress induced polymer migration, a phenomenon very important to the translational diffusion of polymer molecules in nonhomogeneous flows, especially, near the wall. Detailed analyses on the mathematical structure of the model as well as the rheological consequence of the effect are currently summarized in a preprint.

An approximate theory for uniaxial molecules is being examined with appropriate parameters to evaluate the effect of molecular stretching on the rheological behavior of the flowing material. Experimental rheologists has long suspected that the conformational change of LCP molecules in the flow may have been one of the key ingredients that has been missing in the rigid rod or disk models for LCPs. With this new model, we can capture the three distinctive viscosity regime, eluded the previous lcp theories. We hope we will be able to give more detailed explanations for this speculation soon. Ref [1,2,8,12,22,28].

Material property characterization through mesoscopic structure calculations

Through interaction with Dr Vaia at WPAFB and joined by Prof. Lipton of LSU, we carried out a series study on the conductivity property of polymer-particle-inclusion nanocomposites. We employed a homogenization technique to arrive at the effective conductivity property of the nanocomposites described by the mesoscopic structure tensor of the nanocomposites. The mesoscopic structure is the output of our nonhomogeneous theory for nanocomposites. The conductivity properties at various material parameter regimes are investigated. Spatially inhomogeneous morphology of the nanocomposites is explored recently giving rise to an effective medium property throughout the physical domain where the medium resides. Ref [19,21,23,27].

Modeling incompressible fluids through continuum mechanics principles

This is a joint work with Prof. Stephen Bechtel of Ohio State and Frank Rooney. In a continuing effort to model incompressible fluids with prescribed density variations, we examined the models we developed for incompressible fluids with various prescribed density variations through mechanics principles. We clarified the definition of the pressure for these types of constraint theories and studied the flow and temperature profiles in plane Couette and Poiseuille flows. The results are published in International Journal of Engineering Science and Physics of Fluids. Ref [14, 17].

Multiscale kinetic theories for flows of Biaxial liquid crystal polymers

Given the rising interests in the modeling of nanofluids of biaxial constituents such as the flow of liquid crystal polymers, we developed a hydrodynamic theory for the biaxial liquid crystal polymer by modeling it as an ellipsoid suspended in viscous solvent. The excluded volume interaction potential is calculated from the first principle. Detailed analysis is underway and will be reported in the next annual report to AFOSR.

Permeation mode in weak flows of cholesteric liquid crystal polymers

We have obtained the mesoscopic structure using a coarse-grained approximation and homogenization technique for very small pitch cholesterics. We obtained the order parameter variation across the flow field as well as their influence to the major director orientation in the flow. The work has been submitted to DCDS-series B and J. of Non-Newtonian Fluid Mechanics (2005). Ref [28,29].

On-going projects

We are in the process of preparing submissions on our work about the monodomain dynamical study of models for lcp molecules of finite extensibility and mesostructure simulation of nonhomogeneous lcps with density variations. Our 3-D code for the simulation of shear nematic rigid polymers is in the process to be parallelized and run on super-computers.

The research activities on the projects funded by the award are proceeding smoothly according to the plan. Additional projects closely related to the original proposed are identified and added to our research activities. We anticipate the slightly expanded scope of research will facilitate our efforts for the overall objective as well as meet the need of the Air Force. We will report out progress on the on-going projects in our next technical report.

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BOOK CHAPTERS

34. Q. Wang, "Constitutive Modeling of Complex Fluids: Flexible Polymers and Liquid Crystalline Polymers", to appear in Lecture Notes on Complex Fluids, edited by J. Liu and C. Liu, World Scientific, 2005.